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Proton chemical shifts and three-dimensional structure of seven-membered ring 1,3,2-dioxaheterocycles and their six-membered ring heteroanalogs

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Abstract

1. A theoretical basis has been provided for the demonstrated experimental principles in series of seven-membered ring, partially fixed, 1,3,2-dioxaheterocycles and their six-membered ring heteroanalogs, the theoretical foundation makes it possible to correlate proton chemical shifts and conformational structures of the heterocycles in question. 2. An approach has been used here for the first time, based on simultaneous analysis of experimental data for related compounds and theoretical calculations of expected changes in magnetic shielding arising from the influence of fragments with random symmetry. © 1988 Plenum Publishing Corporation.

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